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Structures and properties of uranium–niobium intermetallic compounds under high pressure: A first principles study

Nanyun Bao
;

Qunchao Tong;

Fangyu Guo
;

Shen Zhang;

Dongdong Kang
;

Akinwumi Akinpelu
;

Jian Lv;

Yansun Yao

;

Jiayu Dai

Author & Article Information

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Metallic uranium-based alloys, with *d*-transition metals such as Nb, Mo, and Zr, are promising candidates for actinide fuel. For this purpose, their behaviors under changing physical stimuli need to be understood. Here, we systematically investigate U–Nb intermetallic compounds and predict new compound formations under different pressures using the first-principles swarm-intelligence structure searching method. Two new compounds (U_1Nb_6 and U_2Nb_1) were identified to be thermodynamically stable at ambient and high pressures. U_1Nb_6 has a triclinic symmetry that is stable in the pressure range of 0–200 GPa, while U_2Nb_1 has a hexagonal closely packed structure at low pressure and transforms to a simple hexagonal lattice at 20 GPa. Other compounds, particularly U-rich ones (U_3Nb_1, U_4Nb_1, U_5Nb_1, and U_6Nb_1), are found metastable at ambient and high pressures, and all have orthorhombic structures. The structural, vibrational, electronic, and mechanical properties of predicted U-rich compounds were thoroughly studied using density-functional theory. The results of phonon spectra and elastic constant show that the predicted new structures are dynamically and mechanically stable in the corresponding pressure range. Also, these newly identified U-rich compounds exhibit strong composition dependence, and the pressure-induced enhancements of structural stability and mechanical performances are evident. These

findings shall enrich the understanding of U-based alloys and serve as meaningful predictions for experimental research in the future.

Topics

Density functional theory, **First-principle calculations**, **Phase transitions**, **Elastic modulus**, **Materials properties**, **Chemical elements**, **Crystal lattices**, **Crystal structure**, **Phonon spectroscopy**, **Stoichiometry**

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